**Your Name**:

07/16/2012

**Paper 1 – Aldo**

Cho, Y.; Ioerger, T.; Sacchettini, J., Discovery of novel nitrobenzothiazole inhibitors for Mycobacterium tuberculosis ATP phosphoribosyl transferase (HisG) through virtual screening. *J Med Chem* **2008,** *51* (19), 5984-92.

Question 1: What are two reasons that HisG is a particularly good target?

Answer:

Question 2: In paragraph 1, it says that the pathway is regulated by allosteric inhibition. So, how can they do virtual screening on this target if it is not competitive inhibition?

Answer:

Question 3: What are knockout studies and why are they beneficial to this specific work?

Answer:

Question 4: In Figure 1, circle what is transferred in the reaction.

Answer:

Question 5: When designing virtual screening expts for this target, which substrate site would be best to make your ligands fit into?

Answer:

Question 6: In figure 4 – which ligand is the best inhibitor?

Answer:

Question 7: In Figure 5, write down the IC50 for each compound next to each image. Can you explain why they differ? Which ligand is best and why?

Answer: